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Lipid Processing Technology: Shifting From Waste Streams to High-Value Commercial by-Products

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In the last decades of the 20th century, a powerful international industry based largely on petroleum feedstock arose. This situation was driven mainly by the chemical industry that focused its production and research efforts on commodity chemicals. However, this situation has changed over the last few years. Nowadays, consumer needs and preferences for products based on performance have led the chemical industry to evolve beyond commodities toward specialty chemicals and 'consumer oriented chemicals based products'. Even though petroleum-based products are still ahead in world markets, the available market niche for these innovative products is not a constraint to them or to pharmaceutical products. Products obtained from renewable sources (e.g. vegetable oils and fats) have gained significance as the needs for healthier food products or the growing interest in biofuels, among others, have increased in the last decade. Regrettably, the oleochemical industry is far behind the chemical industry in terms of thermophysical property modeling and development of computational tools suitable for the design, analysis, and optimization of lipid-related processes.

The aim of this work is to present the development of computer-aided methods and tools for the systematic design, analysis, and simulation of processes/products employing lipid technologies. This includes, the identification and classification of the most representative lipid chemical species found in the edible oil and biodiesel industries and their representation in terms of molecular structure and the buildup of appropriate models for estimating pure component properties needed for model-based design and analysis of edible oil and biodiesel processes. In addition, for the modeling of phase behavior of relevant lipid mixtures, a combined group-contribution and atom connectivity approach (Group-Contribution^{Plus} (GC^{Plus})) that is able to extend the application range of property models has been developed. The main idea is the use of connectivity indices to describe the molecular fragmentation that relates properties which is the molecular interactions with the molecular structures.

For this purpose, a filled lipid-database (CAPEC_Lipids_Database) of collected experimental data from the open literature, confidential data from industry and generated data from validated predictive property models; as well as modeling tools for fast adoption-analysis of property prediction models to make it suitable for application with other computer-aided tools was developed. The CAPEC_Lipids_Database contains a total of 2603 data points collected for 12 pure component properties for a total of 243 lipid compounds. Among them 73 are triglycerides (C31-C63), 41 are diglycerides (C27-C43), 15 are monoglycerides (C11-C17), 29 are free fatty acids (C6:C24), 29 are methyl esters (C7-C25), 29 are ethyl esters (C8-C26), 4 are tocopherols (C27-C29), 4 are tocotrienols (C27-C29), 9 are terpenes (C30-C40), and 8 are sterols (C27-C53). For single value pure component properties and temperature dependent properties such as vapor pressure, enthalpy of vaporization, heat capacity, liquid viscosity, and surface tension GC-based models fine-tuned for the lipid chemicals were employed; in the case of the liquid density, the well-known modified Rackett equation and the Chemical Constituent Fragment approach were used. The regression of the adopted GC-based model parameters needed experimental data. PC-SAFT EoS was used to generate pseudo-experimental data when real data was not available. For the modeling of phase behavior of the relevant lipid mixtures, a master parameter table that contains all the needed binary interaction parameters fine tuned for lipid chemicals is made available. A user-added database (CAPEC_LIPIDS_x.x) that can be directly linked to PRO/II has been generated from the lipid-database. Through this database, PRO/II can be used to simulate and optimize edible oil process flowsheets.

Finally, the applicability of the developed methods and tools is shown through the analysis and simulation of the physical refining process of oils and fats. Within the traditional oleochemical industry this process is quite interesting because apart from obtaining the final oil product, it can now be employed to also produce (extract and refine) the high-value commercial by-products such as

tocopherols and sterols.

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